

Magnetic properties of an exchange-coupled biferromagnetic interface

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The theory of an exchange-coupled biferromagnetic interface is developed within the spin-wave approximation. The Green's function for such an interface is derived and used to evaluate the magnetic properties of the interface. It is shown that under certain circumstances either 0, 1, or 2 branches of interface magnons may exist. These magnons exist either above the bulk subbands of the two ferromagnets forming the interface or inside the gap, if such a gap exists. The low-temperature behavior of the interface magnetization is derived and is shown to depend on the bulk properties of the two ferromagnets only.

I. INTRODUCTION

The study of localized excitation modes at the planar interface, formed between two crystals, is a relatively new branch of surface physics. Like many other studies in this field it is stimulated by recent progress in the experimental techniques. In particular, the method of molecular-beam epitaxy enables one to obtain well-defined registered interfaced bicrystals.^{1,2} The existence of such interfaces leads, under certain circumstances, to the existence of interface states. These are states bound in the directions perpendicular to the interface and wavelike parallel to it. Bound interface electronic states were considered recently by several authors, including Yaniv,³ Davison and Cheng,⁴ Muscat, Lannoo, and Allan,⁵ and by Lowy and Madhukar.⁶ In addition to these single-particle excitations, the collective excitations of such interfaces were also studied. For example, one can mention topics such as the vibrational properties and the existence of interface phonons which were discussed by several authors, e.g., Djafari-Rouhani and Dobrzynski,⁷ Djafari-Rouhani, Dobrzynski, and Wallis,⁸ and Masri.⁹ The effects of the Coulomb interelectronic interaction, leading to the presence of interface plasmons, were considered by Stern and Ferrell,¹⁰ Miller and Axelrod,¹¹ Kunz,¹² and Forstmann and Stenschke.¹³

More recently, the present author¹⁴ has developed the macroscopic theory of biferromagnetic interface magnons in dipolar ferromagnets. The present work is a contribution to the microscopic theory of the magnetic excitations and the magnetic structure of an exchange coupled biferromagnetic interface. The system we consider is composed of two Heisenberg ferromagnets coupled via a nearest-neighbor interface exchange coupling. The corresponding physical system we have in mind is an interface of two

Heisenberg ferromagnets grown epitaxially one on top of the other. The properties of this system are analyzed within the Green's function formalism, completely analogous to the one employed by us in our study of the bimetallic interface.³ The explicit model of the interface is presented in Sec. II. The corresponding Green's function is derived in Sec. III. This Green's function is used in Sec. IV to analyze the conditions under which interface magnons exist. In Sec. V we discuss the low-temperature interface magnetization.

II. THE INTERFACE MODEL

The system considered in the present work is a (100) registered interface formed between two Heisenberg ferromagnets, each one having a simple-cubic structure. The spins on the two sides of the interface are coupled through a nearest-neighbor exchange interaction. We assume that the corresponding exchange integral J_{12} is positive, and that the ground state of the combined crystal is a ferromagnetic ground state. In the following we consider the properties of the ferromagnetic interface in the absence of an external magnetic field. The effects of such a field can be taken into account in a simple way.

The Hamiltonian of the interfaced crystal is assumed to be a Heisenberg-type Hamiltonian

$$\mathcal{H} = - \sum'_{\vec{m} \neq \vec{n}} J_{\vec{m}, \vec{n}} \vec{S}_{\vec{m}} \cdot \vec{S}_{\vec{n}}, \quad (2.1)$$

where $\vec{S}_{\vec{m}}$ is the local-spin operator at the lattice site \vec{m} , and $J_{\vec{m}, \vec{n}} > 0$ is the exchange coupling for two spins, one at site \vec{m} and the other at site \vec{n} . The prime on the summation sign in expression (2.1) indicates a summation over nearest-neighbors (NN) sites only. In the following we shall use the one-

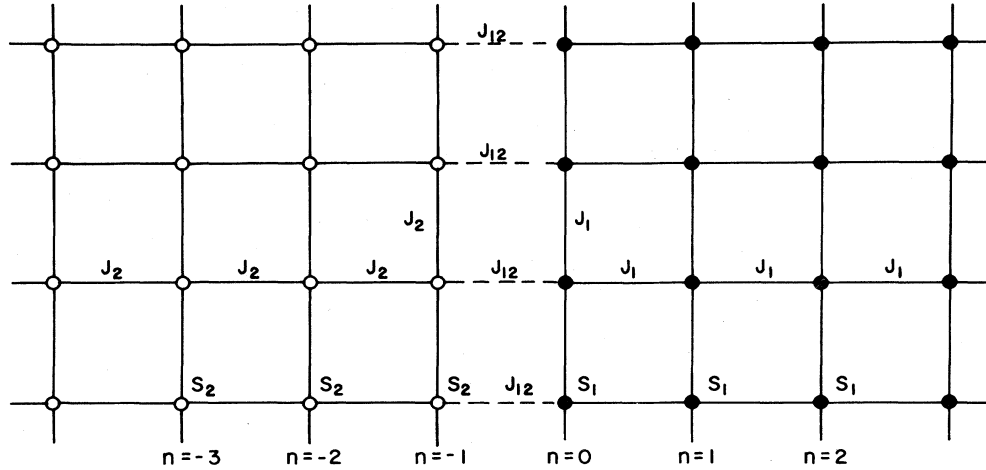


FIG. 1. Schematic representation of the ferromagnetic interface considered in the present work. The two ferromagnets are characterized by spins S_1 and S_2 and exchange constants J_1 and J_2 , respectively. The interface coupling is J_{12} .

dimensional index n to denote the various spin layers parallel to the interface. This index is defined in such a way that the planes $n=0,1,2,\dots$, are occupied by type-1 spins, whereas the planes $n=-1,-2,-3,\dots$, are occupied by type-2 spins. In this notation the interface is formed between the planes $n=0$ and $n=-1$. Spins which belong to these interface layers interact via the interface exchange coupling J_{12} whereas the other spins interact via the corresponding bulk interactions. Thus, the exchange parameter $J_{\vec{m},\vec{n}}$ in expression (2.1) is given by

$$J_{\vec{m},\vec{n}} = \begin{cases} J_1 \\ J_2 \\ J_{12} \end{cases} \quad (2.2)$$

if \vec{m} and \vec{n} are type-1 NN spins, if \vec{m} and \vec{n} are type-2 NN spins, and if \vec{m} and \vec{n} are NN on opposite sides of the interface, respectively. A schematic description of the interface considered here is shown in Fig. 1. The Hamiltonian (2.1) can be expressed in the usual way in terms of the operators $S_{\vec{n}}^{\pm} = S_{\vec{n}}^x \pm iS_{\vec{n}}^y$. These operators can be replaced, within the spirit of the spin-wave approximation, by

$$\vec{a}_{\vec{n}}^{\dagger} \simeq \frac{S_{\vec{n}}^{-}}{(2S_{\vec{n}})^{1/2}}, \quad a_{\vec{n}} \simeq \frac{S_{\vec{n}}^{+}}{(2S_{\vec{n}})^{1/2}}, \quad (2.3)$$

where $a_{\vec{n}}^{\dagger}$ ($a_{\vec{n}}$) creates (destroys) a local-spin deviation at site \vec{n} , and $S_{\vec{n}}$ is the magnitude of the corresponding local spin. The operators $a_{\vec{n}}^{\dagger}$, $a_{\vec{m}}$ obey the usual Boson commutation relations. In terms of these operators the z component of the corresponding spin operators are given by the well-known expression

$$S_{\vec{n}}^z = S_{\vec{n}} - a_{\vec{n}}^{\dagger} a_{\vec{n}}. \quad (2.4)$$

We note that the spin magnitude $S_{\vec{n}}$ in Eqs. (2.3) and (2.4) is either S_1 or S_2 depending on whether \vec{n} is a lattice site to the right or to the left of the interface, respectively.

In treating the bulk properties of a ferromagnet it is advantageous to use the translational symmetry and transform from the site representation $a_{\vec{n}}^{\dagger}$ to the spin-wave representation $a_{\vec{k}}^{\dagger}$, where \vec{k} is the corresponding wave vector, confined to the first Brillouin zone (BZ). For the interface considered in the present work only translations parallel to the interface are symmetry operations. As a result of this symmetry, the crystal momentum parallel to the interface, k_{\parallel} , is still a good quantum number. \vec{k}_{\parallel} spans the two-dimensional Brillouin zone defined by the combined crystal symmetry parallel to the interface. Owing to the reduced symmetry of the interface problem it is convenient to work in a mixed representation which is localized on planes parallel to the interface. We define the spin-deviation creation and destruction operators, on a given plane n with a given transverse crystal momentum \vec{k}_{\parallel} , by

$$a_{\vec{k}_{\parallel},n}^{\dagger} = N_{\parallel}^{-1/2} \sum_{\vec{n}_{\parallel}} e^{-i\vec{k}_{\parallel} \cdot \vec{n}_{\parallel}} a_{\vec{n}}^{\dagger}, \quad (2.5)$$

$$a_{\vec{k}_{\parallel},n} = N_{\parallel}^{-1/2} \sum_{\vec{n}_{\parallel}} e^{i\vec{k}_{\parallel} \cdot \vec{n}_{\parallel}} a_{\vec{n}},$$

where n and \vec{n}_{\parallel} denote the perpendicular and the parallel components of \vec{n} relative to the interface, respectively.

Keeping terms of up to second order in the planar spin-deviation creation and destruction operators (2.5), we can express the interface Hamiltonian (2.1) as follows:

$$\mathcal{H} = \mathcal{H}_1^0 + \mathcal{H}_2^0 + \Delta\epsilon_0 + V. \quad (2.6)$$

In this expression \mathcal{H}_1^0 and \mathcal{H}_2^0 are, respectively, the spin Hamiltonians of a semi-infinite system of type-1 and type-2 Heisenberg spins. These Hamiltonians describe the surface properties of the two ferromagnets considered within the spin-wave approximation. The third contribution $\Delta\epsilon_0$, to the interface Hamiltonian (2.6), gives the change in the ground-state energy due to the formation of the interface from the two semi-infinite systems. It is a c number, given by

$$\Delta\epsilon_0 = -N_{\parallel} J_{12} S_1 S_2, \quad (2.7)$$

where N_{\parallel} is the number of spins in a plane parallel to the interface. Since $\Delta\epsilon_0$ is a constant term, it does not play any role in determining the dynamic properties of the system, and will thus be disregarded in the following. The last term in the interface Hamiltonian (2.6) describes the coupling between the two semi-infinite ferromagnets, which is responsible for the creation of the interface.

In the planar representation it is given by

$$V = 2J_{12} \sum_{\vec{k}_{\parallel}} (S_1 a_{\vec{k}_{\parallel}, -1}^{\dagger} a_{\vec{k}_{\parallel}, -1} + S_2 a_{\vec{k}_{\parallel}, 0}^{\dagger} a_{\vec{k}_{\parallel}, 0}) - 2J_{12} (S_1 S_2)^{1/2} \sum_{\vec{k}_{\parallel}} (a_{\vec{k}_{\parallel}, 0}^{\dagger} a_{\vec{k}_{\parallel}, -1} + a_{\vec{k}_{\parallel}, -1}^{\dagger} a_{\vec{k}_{\parallel}, 0}). \quad (2.8)$$

The existence of an exchange coupling between the spins on the planes $n=0$ and $n=-1$ gives rise to two effects. The first one is equivalent to an effective local magnetic field at the interface layers $n=0$ and $n=-1$. This effect is described by the diagonal terms in the perturbation (2.8). The second effect is the possibility of transferring spin deviations from one side of the interface to the other. This process, which is described by the off-diagonal terms of (2.8), has an amplitude of $-2J_{12}(S_1 S_2)^{1/2}$.

Obviously, since \vec{k}_{\parallel} is a good quantum number, V is diagonal in \vec{k}_{\parallel} . This is true for any matrix element of the interface Hamiltonian. Therefore, we can suppress the explicit \vec{k}_{\parallel} dependence of the various quantities. In this way we define the set of states $\{|n\rangle\}$, localized around the planes $\{n\}$, as the set of states obtained from the ferromagnetic ground state by the application of the spin-deviation creation operators $a_{\vec{k}_{\parallel}, n}^{\dagger}$, with a given \vec{k}_{\parallel} . As Eq. (2.8) shows, the only nonvanishing matrix elements of the interface perturbation are diagonal in \vec{k}_{\parallel} and are given by

$$\langle 0 | V | 0 \rangle \equiv V(0, 0) = 2J_{12} S_2, \quad (2.9a)$$

$$\langle -1 | V | -1 \rangle \equiv V(-1, -1) = 2J_{12} S_1, \quad (2.9b)$$

$$\langle -1 | V | 0 \rangle \equiv V(-1, 0) = -2J_{12} (S_1 S_2)^{1/2}, \quad (2.9c)$$

$$\langle 0 | V | -1 \rangle \equiv V(0, -1) = -2J_{12} (S_1, S_2)^{1/2}. \quad (2.9d)$$

Thus, the interface perturbation is localized around the planes $n=0$ and $n=-1$ within the planar representation.

III. THE FERROMAGNETIC INTERFACE GREEN'S FUNCTION

To obtain the interface Green's function we start from the bulk systems. Introducing the necessary perturbation we then create the corresponding semi-infinite surface systems of the two ferromagnets. At this stage we apply the exchange coupling between the two surfaces and form the ferromagnetic interface.

The energies of the bulk magnons in the exchange coupled ferromagnets considered here are given by the well-known expression

$$\epsilon(\vec{k}) = 12JS - 4JS[\cos(k_z a) + \Lambda(\vec{k}_{\parallel})], \quad (3.1)$$

where a is the lattice constant, and

$$\Lambda(\vec{k}_{\parallel}) = \cos(k_x a) + \cos(k_y a). \quad (3.2)$$

As \vec{k}_{\parallel} spans the two-dimensional Brillouin zone, Λ varies between -2 and $+2$. The Green's function of the single-particle Hamiltonian \mathcal{H} is defined by

$$(E - i\eta - \mathcal{H})G = 1, \quad (3.3)$$

where $\eta = +0$. Since the various Green's function, considered here, are diagonal within the mixed representation, we shall omit the corresponding δ function $\delta_{\vec{k}_{\parallel}, \vec{k}'_{\parallel}}$ and use the notation $G(m, n; \vec{k}_{\parallel})$ for the respective Green's function between states localized around the planes m and n . To simplify the notation we also omit the explicit \vec{k}_{\parallel} dependence. In this way, the bulk Green's function is given by

$$G^0(m, n) = G^0(m - n) = N_{\perp}^{-1} \sum_{k_z} \frac{e^{i(m-n)k_z a}}{E - i\eta - \epsilon(\vec{k})}, \quad (3.4)$$

where N_{\perp} is the number of atomic planes perpendic-

ular to the (001) axis. The summation in expression (3.4) can be performed to yield¹⁵

$$G^0(n) = \frac{i}{\mu} \left[\frac{\omega + i\mu}{-4JS} \right]^{|n|}, \quad (3.5)$$

where

$$\omega = E - 12JS + 4JS\Lambda(\vec{k}_{\parallel}) \quad (3.6)$$

and

$$\begin{aligned} \mu &= (16J^2S^2 - \omega^2)^{1/2} \quad \text{for } \omega^2 \leq 16J^2S^2 \\ &= i \operatorname{sgn}(\omega)(\omega^2 - 16J^2S^2)^{1/2} \quad \text{for } \omega^2 > 16J^2S^2. \end{aligned} \quad (3.7)$$

Here $\operatorname{sgn}(\omega)$ denotes the sign of ω .

To create the surface system from the bulk one, we break the exchange bonds between neighboring spins on the planes $n = -1$ and $n = 0$. Breaking these bonds creates effective magnetic fields at the surface layers $n = 0$ and $n = -1$. In addition, it also changes the transfer amplitude between the corresponding surface layers. The corresponding perturbation described above, is given in the mixed representation by

$$V(0, -1) = V(-1, 0) = 2JS, \quad (3.8a)$$

$$V(0, 0) = V(-1, -1) = -2JS. \quad (3.8b)$$

For reasons that will become clear in the following, we shall solve the surface problem for an arbitrary value of the surface diagonal perturbation, which we denote by U , i.e.,

$$U \equiv V(0, 0) = V(-1, -1). \quad (3.9)$$

The surface Green's function $G(m, n)$ is related to bulk Green's function (3.5) and the perturbation (3.8) via Dyson's equation

$$G = G^0 + G^0VG. \quad (3.10)$$

After solving this equation we find that the surface Green's function is given by

$$\begin{aligned} G(m, n) &= \frac{i}{\mu} \left[\left[\frac{\omega + i\mu}{-4JS} \right]^{|m-n|} \right. \\ &\quad \left. + \left[\frac{\omega + i\mu}{-4JS} \right]^{m+n} \frac{i\mu + (\omega - 2U)}{i\mu - (\omega - 2U)} \right] \end{aligned} \quad (3.11a)$$

$$G(m, m) = G^0(m, m) + 4J_{12}^2 S_1 S_2 G^0(-1, -1) G^0(m, 0) G^0(0, m) [1 - 4J_{12}^2 S_1 S_2 G^0(0, 0) G^0(-1, -1)]^{-1} \quad (3.13a)$$

for $m \geq 0$, and

$$G(m, m) = G^0(m, m) + 4J_{12}^2 S_1 S_2 G^0(0, 0) G^0(m, -1) G^0(-1, m) [1 - 4J_{12}^2 S_1 S_2 G^0(0, 0) G^0(-1, -1)]^{-1} \quad (3.13b)$$

for $m, n \geq 0$,

$$\begin{aligned} G(m, n) &= \frac{i}{\mu} \left[\left[\frac{\omega + i\mu}{-4JS} \right]^{|m-n|} \right. \\ &\quad \left. + \left[\frac{\omega + i\mu}{-4JS} \right]^{|m| + |n| - 2} \right. \\ &\quad \left. \times \frac{i\mu + (\omega - 2U)}{i\mu - (\omega - 2U)} \right] \end{aligned} \quad (3.11b)$$

for $m, n \leq -1$, and

$$G(m, n) = 0 \quad (3.11c)$$

otherwise.

Our final step in the creation of the interface is to take two semiinfinite systems described by (3.11) and introduce the coupling (2.9) between them. As we have seen before, this coupling has diagonal terms, acting on the interface layers $n = 0$ and $n = -1$ and off-diagonal terms which couple the two layers. We apply first the diagonal perturbation. Since we have solved the surface problem for an arbitrary value of the surface perturbation U , this amounts only to a change in the value of this parameter from its original surface value (3.8b) by an amount given by (2.9a) and (2.9b). Thus, the diagonal terms on the two sides of the interface are given by

$$U_1 = -2J_1 S_1 + 2J_{12} S_2, \quad (3.12a)$$

$$U_2 = -2J_2 S_2 + 2J_{12} S_1. \quad (3.12b)$$

The corresponding Green's function obtained after the application of the diagonal perturbation is given by Eq. (3.11a), with ω and μ calculated in terms of J_1 and S_1 and $U = U_1$ for $m, n \geq 0$, by Eq. (3.11b) calculated with $J = J_2$, $S = S_2$, and $U = U_2$ for $m, n \leq -1$, and by (3.11c) otherwise.

We next apply the off-diagonal perturbation (2.9c) and (2.9d) and solve the corresponding Dyson's equation for the diagonal matrix elements of the interface Green's function. In this way we obtain

for $m \leq -1$. In these equations G^0 is the surface Green's function, with the interface value of U_1 and U_2 . When the expressions (3.11) are substituted into (3.13), we obtain the following explicit expressions for the interface Green's function:

$$G(m, m) = \frac{i}{\mu_1} + \frac{1}{\mu_1 + i(\omega_1 - 2U_1)} \left[\frac{\omega_1 + i\mu_1}{4J_1 S_1} \right]^{2m} \times \left[\frac{i\mu_1 + (\omega_1 - 2U_1)}{\mu_1} - \frac{32J_{12}^2 S_1 S_2 i}{16J_{12}^2 S_1 S_2 + [\mu_1 + i(\omega_1 - 2U_1)][\mu_2 + i(\omega_2 - 2U_2)]} \right] \quad (3.14a)$$

for $m \geq 0$, and

$$G(m, m) = \frac{i}{\mu_2} + \frac{1}{\mu_2 + i(\omega_2 - 2U_2)} \left[\frac{\omega_2 + i\mu_2}{4J_2 S_2} \right]^{2|m| - 2} \times \left[\frac{i\mu_2 + (\omega_2 - 2U_2)}{\mu_2} - \frac{32J_{12}^2 S_1 S_2 i}{16J_{12}^2 S_1 S_2 + [\mu_1 + i(\omega_1 - 2U_1)][\mu_2 + i(\omega_2 - 2U_2)]} \right] \quad (3.14b)$$

for $m \leq -1$. In these expressions, the indices 1 and 2 denote parameters evaluated with $J=J_1$, $S=S_1$ and $J=J_2$, $S=S_2$, respectively.

Equation (3.14) is our final expression for the exchange coupled biferromagnetic interface Green's function. It has to be noted that more complicated effects than those considered here can also be taken into account in a similar way. For example, one can allow for a change in the exchange constant for spins on the interface layers $n=0$ or $n=-1$. If ΔJ_1 denotes the deviation of the exchange parameter for two spins on the interface layer $n=0$ from the corresponding bulk value, and ΔJ_2 denotes the respective quantity for spins on the $n=-1$ layer, then the interface Green's function is still given by expression (3.14), but with the following value for U_1 and U_2 :

$$U_1 = -2J_1 S_1 + 2J_{12} S_2 + 4\Delta J_1 S_1 [2 - \Lambda(\vec{k}_{||})], \quad (3.15a)$$

$$U_2 = -2J_2 S_2 + 2J_{12} S_1 + 4\Delta J_2 S_2 [2 - \Lambda(\vec{k}_{||})], \quad (3.15b)$$

where $\Lambda(\vec{k}_{||})$ is given by Eq. (3.2). In the following, such changes in the exchange constants of spins on

the interface layers will be ignored, and we shall use the simpler expressions (3.12) for U_1 and U_2 .

IV. INTERFACE MAGNONS

We turn now to examine the structure of the magnetic excitations of the interface. To this end we shall apply the Green's function derived in the preceding section. From the explicit expressions (3.14a) and (3.14b) it follows that for a fixed $\vec{k}_{||}$, the diagonal matrix elements of the interface Green's function have a nonvanishing, continuous, imaginary part for energies which are either inside the bulk magnon band of the first or the second ferromagnet forming the interface. Since this imaginary part is proportional to the local magnon density of states, it follows that the magnon bandwidth of the biferromagnet is at least the union of the magnon bands of the two separate ferromagnets. As follows from Eq. (3.14), the magnon wave functions of the combined crystal can be classified into three groups, according to their localization properties with respect to the interface.

To facilitate our further analysis we define the $\vec{k}_{||}$ subbands of the two ferromagnets considered. These subbands span the energy range over which the cor-

responding bulk magnons energy varies for a fixed \vec{k}_{\parallel} . These subbands are described by the intersection of the bulk magnon spectra $\epsilon_1(\vec{k})$ and $\epsilon_2(\vec{k})$, Eq. (3.1), where the plane \vec{k}_{\parallel} equals a constant.

The various magnon wave functions of the combined crystal can be labeled by their \vec{k}_{\parallel} value. The first type of these wave functions extends throughout the entire bicrystal. As can be seen from Eq. (3.14), this kind of behavior is associated with states whose energy lies inside the \vec{k}_{\parallel} subbands of both ferromagnets, i.e., those energies satisfying

$$\begin{aligned} |E - 12J_1S_1 + 4J_1S_1\Lambda(\vec{k}_{\parallel})| &< 4J_1S_1, \\ |E - 12J_2S_2 + 4J_2S_2\Lambda(\vec{k}_{\parallel})| &< 4J_2S_2. \end{aligned} \quad (4.1)$$

The second type of magnon wave functions extend to infinity on one side of the interface only, and decay exponentially with the distance from the interface on the other side. Such kind of behavior occurs for energies which are inside the \vec{k}_{\parallel} subband of one of the ferromagnets, but outside the corresponding subband of the other. In this way, magnons whose energy and wave vector satisfy

$$\begin{aligned} |E - 12J_1S_1 + 4J_1S_1\Lambda(\vec{k}_{\parallel})| &< 4J_1S_1, \\ |E - 12J_2S_2 + 4J_2S_2\Lambda(\vec{k}_{\parallel})| &> 4J_2S_2 \end{aligned} \quad (4.2)$$

extend to infinity on the right-hand side of the interface, but decay exponentially on its left-hand side. The reverse situation occurs for energies satisfying

$$\begin{aligned} |E - 12J_1S_1 + 4J_1S_1\Lambda(\vec{k}_{\parallel})| &> 4J_1S_1, \\ |E - 12J_2S_2 + 4J_2S_2\Lambda(\vec{k}_{\parallel})| &< 4J_2S_2. \end{aligned} \quad (4.3)$$

The third, and most interesting, are the interface magnons. These are magnetic excitations whose wave function is exponentially localized on both sides of the interface. As will be shown soon, the existence of such excitations depends on the value of the parameters characterizing the interface. For a given \vec{k}_{\parallel} , the energy of the possible bound interface magnons is determined by the poles of the interface Green's function, which lie outside the \vec{k}_{\parallel} subbands of the two ferromagnets. Applying the explicit expression (3.14) we see that the possible interface magnon energies are given by the roots of the equation

$$\begin{aligned} 16J_{12}^2S_1S_2 - [\text{sgn}(\omega_1)\bar{\mu}_1 + \omega_1 - 2U_1] \\ \times [\text{sgn}(\omega_2)\bar{\mu}_2 + \omega_2 - 2U_2] = 0. \end{aligned} \quad (4.4)$$

In this equation

$$\bar{\mu} = (\omega^2 - 16J^2S^2)^{1/2}, \quad (4.5)$$

and U_1 and U_2 are given by (3.12).

The analytical solution of the interface magnon equation (4.4) is not possible in general. To get some insight into the nature of these solutions, we shall first use a rather artificial limiting model that can be solved analytically. If one assumes that the two ferromagnets have the same magnetic properties, i.e., $J_1 = J_2$, $S_1 = S_2$, then the interface magnon equation (4.4) reduces to

$$16J_{12}^2S^2 - [\text{sgn}(\omega)\bar{\mu} + \omega + 2JS - 2J_{12}S]^2 = 0. \quad (4.6)$$

This equation has a real solution provided the interface exchange coupling is strong enough. Explicitly, to have an interface magnon we must have

$$J_{12} > J. \quad (4.7)$$

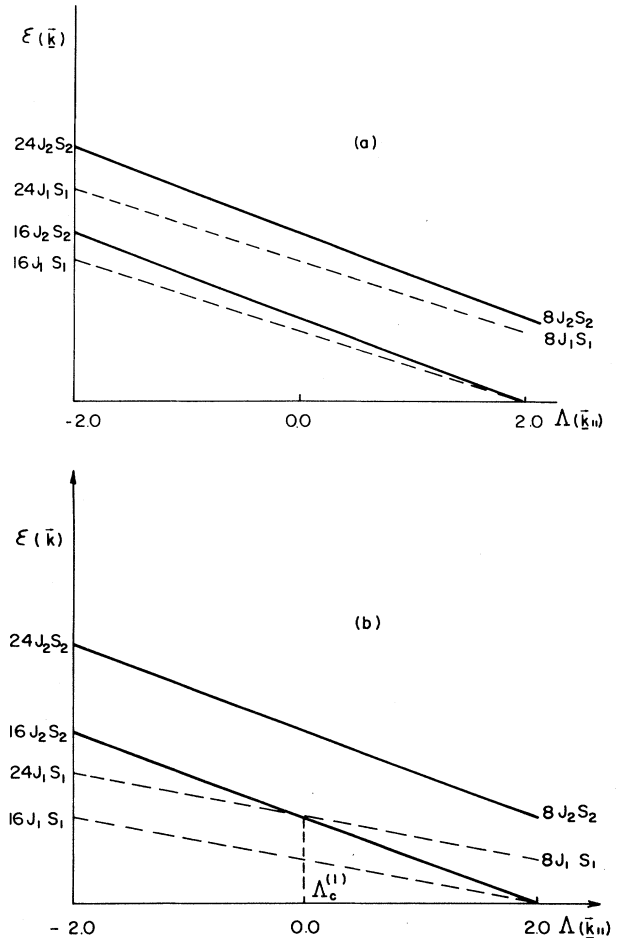


FIG. 2. Bulk magnon structure of the two ferromagnets forming the interface: (a) $\Gamma < \frac{3}{2}$ and (b) $\Gamma > \frac{3}{2}$.

For J_{12} satisfying this relation, an interface magnon branch exists above the bulk \vec{k}_{\parallel} subbands. The energy of this interface magnon is given by

$$E_{\text{in}}(\vec{k}_{\parallel}) = 12JS + 2JS \left[\frac{2J_{12}}{J} - 1 + \frac{1}{2J_{12}/J - 1} \right] - 4JS\Lambda(\vec{k}_{\parallel}). \quad (4.8)$$

As \vec{k}_{\parallel} varies inside the two-dimensional Brillouin zone, $E_{\text{in}}(\vec{k}_{\parallel})$ spans the corresponding interface magnon band. It has to be noted that the existence of a critical value of the interface exchange constant, such as Eq. (4.7), turns out to be a more general property of the interface considered in this work.

We turn now to a qualitative analysis of the general interface magnon equation (4.4). As will be shown in the following, the biferromagnetic interface considered can support either, 0, 1, or 2 interface magnon branches. The specific number of branches is determined by the properties of the two ferromagnets forming the interface, i.e., J_1, J_2 and S_1, S_2 , and by the strength of interface exchange coupling J_{12} . Without any loss of generality we assume in this section that $J_2 S_2 \geq J_1 S_1$, we also introduce the following notations:

$$\Gamma = J_2 S_2 / J_1 S_1, \quad (4.9a)$$

$$\alpha = S_2 / S_1. \quad (4.9b)$$

According to our convention, $\Gamma \geq 1$ in this section. The relative relation of the \vec{k}_{\parallel} subbands of the two

bulk ferromagnets depends on the value of the parameter Γ . For $\Gamma > \frac{3}{2}$ a gap exists between the corresponding \vec{k}_{\parallel} subbands over a certain region of the two-dimensional Brillouin zone. The portion of this zone in which such a gap exists is determined by the requirement

$$\Lambda(\vec{k}_{\parallel}) < \Lambda_c^{(1)}, \quad (4.10a)$$

where

$$\Lambda_c^{(1)} = 2(\Gamma - 2) / (\Gamma - 1). \quad (4.10b)$$

Figure 2 shows the two possibilities, with ($\Gamma > \frac{3}{2}$) and without ($\Gamma < \frac{3}{2}$) a gap between the bulk subbands.

The biferromagnetic interface, considered in the present work, has the general property that for any value of the interface exchange constant $J_{12} > 0$, no interface magnons can appear below the bulk subbands of the two ferromagnets. Such magnons can only exist either above the two subbands or inside the gap between the subbands, when such a gap exists.

We shall consider first the interface magnon branch which lies above the bulk subbands. As a simple graphical analysis shows, no such magnon branch exists if the coupling between the two ferromagnets is too weak. As the coupling constant J_{12} increases, a critical value $J_{12}^{(c1)}$ is reached, above which an interface magnon appears above the two subbands. The value of this critical coupling is \vec{k}_{\parallel} dependent, and is given by

$$J_{12}^{(c1)} = 2J_2\alpha \left[1 - \frac{2\Gamma\alpha}{\{[4\Gamma - 3 - (\Gamma - 1)\Lambda]^2 - 1\}^{1/2} + [2\Gamma(2 + \alpha) - 2 - (\Gamma - 1)\Lambda]} \right]. \quad (4.11)$$

As was noted before, if $\Gamma > \frac{3}{2}$ there exists a gap between the subbands of the two ferromagnets over a certain region of the Brillouin zone. For such cases it is sometimes possible to have interface magnons that lie inside this gap. However, a necessary condition for the existence of such magnons is that the parameters of the two ferromagnets forming the interface should obey

$$[12(2\Gamma - 3)(\Gamma - 1)]^{1/2} + 4\Gamma - 5 > 2/\alpha. \quad (4.12)$$

If this relation is satisfied, there exists a critical interface coupling $J_{12}^{(c2)}$ above which a gap interface magnon will appear. This coupling is given by

$$J_{12}^{(c2)} = \frac{2J_1(\{[4 - 3\Gamma - (1 - \Gamma)\Lambda]^2 - \Gamma^2\}^{1/2} + 2\Gamma - 4 + (1 - \Gamma)\Lambda)}{2 - \alpha(\{[4 - 3\Gamma - (1 - \Gamma)\Lambda]^2 - \Gamma^2\}^{1/2} + 2\Gamma - 4 + (1 - \Gamma)\Lambda)}. \quad (4.13)$$

This gap interface magnon branch exists in the region of the two-dimensional Brillouin zone defined by

$$-2 \leq \Lambda(\vec{k}_{\parallel}) \leq \Lambda_c^{(2)}, \quad (4.14)$$

where $\Lambda_c^{(2)}$ is a solution of the equation

$$\{[4 - 3\Gamma - (1 - \Gamma)\Lambda_c^{(2)}]^2 - \Gamma^2\}^{1/2} - 4 + 2\Gamma + (1 - \Gamma)\Lambda_c^{(2)} - 2/\alpha = 0. \quad (4.15)$$

Thus, if the relation (4.12) is satisfied, and J_{12} is large enough, there will exist two interface magnon branches, one inside the gap and the other above the subbands of the two ferromagnets.

The result that no interface magnons exist below the bulk subbands is specific to the model considered here. It is obvious that if one starts from two semi-infinite subsystems, each having a surface state below the corresponding bulk subband, and couple them via the exchange coupling J_{12} , then the interface system will have an interface magnon branch below the bulk subbands, provided J_{12} is weak enough. Thus the perturbations leading to the presence of surface states below the bulk subbands can lead in the present case to an interface magnon branch below the bulk subbands. These perturbations include, for example, a weakening of the transverse coupling in the interface layers [a negative ΔJ_1 and ΔJ_2 in Eq. (3.15)]. Other situations which can lead in principle to such states are, for example, a higher order interface, where the bonds across the interface are nonperpendicular to it, or a system with a longer range interaction, such as a next-nearest-neighbor (NNN) interaction.¹⁵

It has been noted before that the interface magnons are exponentially localized near the interface. However, the rate of decay of the corresponding wave function is different on the two sides of the interface. Let E_{in} be the energy of the interface magnon considered. The corresponding values of the parameter ω are given by Eq. (3.6), i.e.,

$$\omega_{\text{in}}^{(1)} = E_{\text{in}} - 12J_1S_1 + 4J_1S_1\Lambda(\vec{k}_{\parallel}) , \quad (4.16a)$$

$$\omega_{\text{in}}^{(2)} = E_{\text{in}} - 12J_2S_2 + 4J_2S_2\Lambda(\vec{k}_{\parallel}) . \quad (4.16b)$$

Define now the dimensionless parameters β_1 and β_2 ,

$$\beta_1 = \omega_{\text{in}}^{(1)} / 4J_1S_1 , \quad (4.17a)$$

$$\beta_2 = \omega_{\text{in}}^{(2)} / 4J_2S_2 . \quad (4.17b)$$

These parameters measure the distance of the interface magnon energy from the center of the corresponding \vec{k}_{\parallel} bulk subbands, in terms of half the bulk subbands' widths. It is obvious from our previous discussion that $|\beta_1| > 1$ and $|\beta_2| > 1$. The spatial decay rate of an interface magnon wave function is equal to one-half of the decay rate of the corresponding diagonal Green's function. If we denote by λ_1 and λ_2 the inverse wave-function localization length on the two sides of the interface, respectively, it follows from expression (3.14) that these are given by

$$\lambda_i = -\ln[|\beta_i| - (\beta_i^2 - 1)^{1/2}] , \quad i = 1, 2 . \quad (4.18)$$

Thus the decay rate of an interface magnon is deter-

mined only by its dimensionless distance from the corresponding bulk subband center. The larger this distance is, the more localized is the corresponding interface magnon wave function.

V. THE FINITE TEMPERATURE INTERFACE MAGNETIZATION

As the interface temperature is raised from absolute zero, the local magnetization starts to deviate from its corresponding saturation value. This deviation is given by the thermal average of Eq. (2.4), i.e.,

$$\Delta S_{\bar{n}}^z = \langle a_{\bar{n}}^{\dagger} a_{\bar{n}} \rangle . \quad (5.1)$$

In the case of the interface $\Delta S_{\bar{n}}^z$ depends on the distance of the site \bar{n} from the interface. Let $\rho_n(E)$ be the local density of magnon states at energy E on the plane n . In terms of this density of states, the thermal average (5.1) can be written as follows:

$$\Delta S_n^z = \int_0^{\infty} \rho_n(E) f(E, T) dE , \quad (5.2)$$

where $f(E, T)$ is the Bose-Einstein distribution function. The local density of states $\rho_n(E)$ is related to the interface Green's function (3.14), derived earlier, by

$$\rho_n(E) = \frac{a^2}{\pi} \int \text{Im} G(n, n) \frac{d\vec{k}_{\parallel}}{(2\pi)^2} , \quad (5.3)$$

where Im denotes the imaginary part of a complex function, and the \vec{k}_{\parallel} integration is over the two-dimensional Brillouin zone.

To determine the low-temperature magnetization we have to determine first the local density of magnon states $\rho_n(E)$. At low temperatures the only magnons that contribute to the integral (5.2) are those having a small excitation energy of the order of $K_B T$ where K_B is the Boltzmann constant. These are magnons near the bottom of the bands, in the vicinity of $\Lambda(\vec{k}_{\parallel}) = 2$ (see Fig. 2). As was discussed before, no interface magnons exist below the bulk subbands in the present model. Therefore, their low-temperature contribution to the local magnetization is rather small and can be neglected to leading order in the temperature.

We consider now the local magnon density of states $\rho_n(E)$ near the bottom of the bands. Without loss of generality we assume that $n \geq 0$. Using our general expression (3.14) for the interface Green's function, we can derive the corresponding expression for the local density of states for small E . This expression shows that, depending on the analytic behavior of $\rho_n(E)$ near the bottom of the bands, the system can be divided into three distinct regions. The first is the interface region, given by

$$n \ll \left(\frac{J_1 S_1}{2E} \right)^{1/2}. \quad (5.4)$$

The second is the bulk region, defined by

$$n \gg \left(\frac{J_1 S_1}{2E} \right)^{1/2}. \quad (5.5)$$

The third region is the transition region, between (5.4) and (5.5).

Since the typical magnon energies are of the order of $K_B T$, the division of the system into three regions is actually temperature dependent. At a given temperature T the interface region is given by

$$n \ll \left(\frac{J_1 S_1}{2k_B T} \right)^{1/2}, \quad (5.6)$$

whereas the bulk region is given by

$$n \gg \left(\frac{J_1 S_1}{2k_B T} \right)^{1/2}. \quad (5.7)$$

It follows from our general expressions that the local magnon density of states, near the bottom of the bands, in the interface region (5.4) is given by

$$\rho_n(E) = \rho_0(E) + E^{1/2} O[n(E/J_1 S_1)^{1/2}], \quad (5.8)$$

where $\rho_0(E)$ is the local density of states at the interface layer $n=0$. On the other hand, $\rho_n(E)$ in the bulk region (5.5) is given by

$$\rho_n(E) = \rho_b(E) + O(1/n), \quad (5.9)$$

where $\rho_b(E)$ is the corresponding bulk density of states.

An explicit evaluation shows that the interface density of states (5.8), and the bulk density of states have a similar dependence on the energy. In fact both vary like $E^{1/2}$, but with a different coefficient. This observation allows us to write

$$\rho_0(E) = A_0(\alpha, \Gamma) \rho_b(E), \quad (5.10)$$

in which the quantity A_0 is independent of the energy, and is a function of the parameters α and Γ defined in (4.9). The bulk density of states is given by the well-known expression

$$\rho_b(E) = \frac{E^{1/2}}{(2\pi)^2 (2J_1 S_1)^{3/2}}, \quad (5.11)$$

whereas A_0 is given, for $\Gamma \neq 1$, by

$$A_0(\alpha, \Gamma) = \int_0^1 \frac{(1-z)^{1/2}}{v(z)} dz - \alpha \Gamma^{1/2} \int_0^{1/\Gamma} \frac{(1-\Gamma z)^{1/2}}{v(z)} dz, \quad (5.12)$$

where

$$v(z) = 1 - z + \alpha^2 \Gamma (\Gamma z - 1). \quad (5.13)$$

Substituting expression (5.10) for $\rho_0(E)$ into Eq.

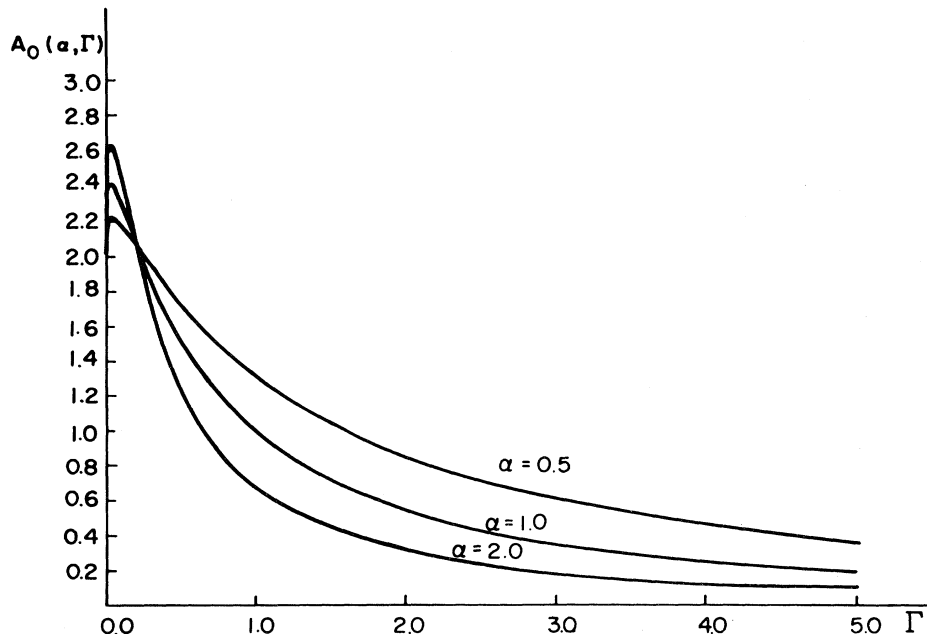


FIG. 3. Interface magnetization enhancement factor as a function of $\alpha = S_2/S_1$ and $\Gamma = J_2 S_2/J_1 S_1$.

(5.2) for the local-spin deviation shows that the interface spin deviation is related to the corresponding bulk-spin deviation by

$$\Delta S_0^z(T) = A_0(\alpha, \Gamma) \Delta S_b^z(T). \quad (5.14)$$

Thus $A_0(\alpha, T)$ is the interface magnetization enhancement factor. It shows by how much the interface spin deviation in the region (5.6) is larger or smaller than the corresponding bulk spin deviation. This bulk spin deviation itself is given by the well-known Bloch's law

$$\Delta S_b^z(T) = \frac{\Gamma(\frac{3}{2})\zeta(\frac{3}{2}; 1)}{(2\pi)^2} \left[\frac{k_B T}{2J_1 S_1} \right]^{3/2}. \quad (5.15)$$

In this expression $\Gamma(x)$ is the gamma function and $\zeta(s, a)$ is the Riemann zeta function.

One can derive an analytic expression for the interface magnetization enhancement factor from Eq. (5.13). The resulting expression is quite cumbersome, and is given therefore in the Appendix. Figure 3 shows the dependence of $A_0(\alpha, \Gamma)$ on Γ for several values of the parameter α . As shown in this figure, the interface magnetization can be either smaller or larger than the corresponding bulk magnetization, depending on the specific parameters of the interface α and Γ .

The results derived in this section lead to the following interesting conclusions:

(a) The bulk and the interface spin deviations have the same temperature dependence. Both increase according to a $T^{3/2}$ rule, but with different coefficients.

(b) As long as the interface coupling J_{12} is finite, the low-temperature interface spin deviation is independent of the strength of the coupling. It is determined only by the bulk properties of the two ferromagnets forming the interface.

The calculation performed up to now was con-

cerned with the right-hand side layers $n \geq 0$, which are occupied by type-1 spins. To obtain the corresponding results for the other ferromagnet forming the interface, i.e., for spins on the layers $n \leq -1$, all we have to do is to change α into α^{-1} and Γ into Γ^{-1} . In this way we have

$$A_{-1}(\alpha, \Gamma) = A_0(\alpha^{-1}, \Gamma^{-1}), \quad (5.16)$$

where A_{-1} is the interface magnetization enhancement factor for the interface region of the spin layers $n \leq -1$.

A final remark that should be added here is that the limiting case of a free surface can be obtained from our model by setting $\Gamma = 0$. In this case we get

$$A_0(\alpha, 0) = 2.$$

This is just the known result,¹⁵ that the free surface spin deviation is twice the corresponding bulk deviation.

APPENDIX

In this appendix we give an explicit expression for the interface magnetization enhancement factor $A_0(\alpha, \Gamma)$. This quantity is given by Eq. (5.12). The two integrals appearing in this equation can be evaluated by noting that both have the formal form

$$\int \frac{\sqrt{u(x)}}{v(x)} dx, \quad (A1)$$

where both $u(x)$ and $v(x)$ are linear forms of x . The integration is performed by transforming to a new variable

$$t = \sqrt{u(x)}. \quad (A2)$$

Depending on the position of the poles of the integrand, we obtain the following expressions:

$$(a) \text{ For } (1 - \Gamma)/(\alpha^2 \Gamma^2 - 1) < 0,$$

$$A_0(\alpha, \Gamma) = \frac{2}{\alpha^2 \Gamma^2 - 1} \left[\alpha \Gamma^{1/2} - 1 + \frac{k}{2} \left[\ln \left| \frac{(\alpha \Gamma^{1/2} - k)(1 + k)}{(\alpha \Gamma^{1/2} + k)(1 - k)} \right| \right] \right], \quad (A3)$$

where

$$k^2 = \frac{\alpha^2 \Gamma(\Gamma - 1)}{\alpha^2 \Gamma^2 - 1}.$$

$$(b) \text{ For } (1 - \Gamma)/(\alpha^2 \Gamma^2 - 1) > 0,$$

$$A_0(\alpha, \Gamma) = \frac{2}{\alpha^2 \Gamma^2 - 1} \left\{ \alpha \Gamma^{1/2} - 1 + k \left[\arctan \left[\frac{1}{k} \right] - \arctan \left[\frac{\alpha \Gamma^{1/2}}{k} \right] \right] \right\}, \quad (A4)$$

where

$$k^2 = \frac{\alpha^2 \Gamma(1-\Gamma)}{\alpha^2 \Gamma^2 - 1}.$$

(c) When $\alpha\Gamma = 1$ we have the simpler expression

$$A_0 \left[\frac{1}{\Gamma}, \Gamma \right] = \frac{2}{3} \Gamma^{1/2} \frac{(1 + \Gamma^{1/2} + \Gamma)}{1 + \Gamma^{1/2}}. \quad (\text{A5})$$

(d) Also when $\alpha^2\Gamma = 1$ we have

$$A_0(\Gamma^{-1/2}, \Gamma) = \frac{\ln \Gamma}{\Gamma - 1}. \quad (\text{A6})$$

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